LA-UR-04-0123

Approved for public release; distribution is unlimited.

Title: Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNP™ Criticality Validation Suite

Author(s): Russell D. Mosteller

Submitted to: 2004 Annual Meeting of the American Nuclear Society June 13 - 17, 2004

Pittsburgh, PA





Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publish cognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this commution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Comparison of ENDF/B-VI and Preliminary ENDF/B-VII Results for the MCNPTM Criticality Validation Suite

Russell D. Mosteller

Applied Physics Division, Los Alamos National Laboratory, Los Alamos, NM, 87545, mosteller@lanl.gov

An initial assessment of the impact of preliminary data proposed for ENDF/B-VII has been made using the MCNP criticality validation suite. Relative to ENDF/B-VI, the data changes primarily involve high-energy elastic and inelastic scattering in the uranium isotopes and ²³⁹Pu, as well as resonance parameters for ²³⁸U.

The criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*. ¹ It contains cases for a variety of fuels, including ²³³U, highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), and plutonium. For each fuel type, there are cases with a variety of moderators, reflectors, spectra, and geometries. The cases in the suite are summarized in Table I.

Three sets of calculations were performed for the suite using the MCNP5 Monte Carlo code.² The first set employed nuclear data from ENDF/B-VI Release 8, the final release for ENDF/B-VI. The second set employed preliminary ENDF/B-VII data generated by group T-16 at Los Alamos National Laboratory for the uranium isotopes and for ²³⁹Pu but retained ENDF/B-VI data for all other nuclides. The third set was the same as the second except that a new set of ²³⁸U resonance

parameters generated by researchers at Oak Ridge National Laboratory (ORNL) was added to the T-16 evaluation.

The MCNP5 calculations were run with 5,000,000 active neutron histories for all but two cases in the suite. Only 3,000,000 active histories were used for those cases, SB-5 and Zebra-8H, because they require substantially more computer time per history than the other cases. Nonetheless, the standard deviation for k_{eff} from those cases is comparable to those for other cases in the suite. The results from these calculations are presented in Table II.

The preliminary ENDF/B-VII data produce marked improvements in $k_{\rm eff}$ for bare spheres of ^{233}U (Jezebel-233), HEU (Godiva), and plutonium (Jezebel and Jezebel-240) as well as the other unreflected HEU and plutonium cases (Tinkertoy02 (c-11) and Pu Buttons, respectively). Furthermore, the reactivity swings between those bare spheres and the corresponding Flattop cases (which enclose the sphere inside an annulus of normal uranium) are substantially decreased. The changes also significantly improve $k_{\rm eff}$ for BIG TEN and for HEU and plutonium spheres immersed in water (Godiver and Pu-MF-11, respectively). In addition, inclusion of the ORNL

Table I. MCNP Criticality Validation Suite.

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
²³³ U	Jezebel-233	Flattop-23	U233-MF-05 (2)*	Falstaff (1) [†]	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	UH ₃ (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H [‡]	IEU-CT-02 (3)	STACY-36
LEU					BaW XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG [‡]	PNL-33	PNL-2

- * Numbers in parentheses identify a specific case within a sequence of benchmarks
- † Extrapolated to critical
- ‡ k measurement

Table II MCNP5 Results for Criticality Safety Validation Set.

				Calculated k _{eff}		
Туре	Spectrum	Case	Benchmark k _{eff}	T-16 + ORNL ²³⁸ U	T-16	ENDF/B-VI
²³³ U	Fast	Jezebel-233 Flattop-23 U233-MF-05 (2)	$\begin{array}{c} 1.0000 \pm 0.0010 \\ 1.0000 \pm 0.0014 \\ 1.0000 \pm 0.0030 \end{array}$	0.9984 ± 0.0003 0.9988 ± 0.0003 0.9964 ± 0.0003	0.9989 ± 0.0002 0.9985 ± 0.0003 0.9968 ± 0.0003	0.9931 ± 0.0002 1.0003 ± 0.0003 0.9976 ± 0.0003
	Intermediate	Falstaff (1)	1.0000 ± 0.0083	0.9876 ± 0.0005	0.9876 ± 0.0005	0.9894 ± 0.0005
	Thermal	SB-2½ ORNL-11	1.0000 ± 0.0024 1.0006 ± 0.0029	0.9948 ± 0.0005 1.0004 ± 0.0002	0.9946 ± 0.0005 1.0002 ± 0.0002	$0.9967 \pm 0.0005 \\ 0.9968 \pm 0.0002$
HEU	Fast	Godiva Tinkertoy-2 (c-11) Flattop-25 Godiver	$\begin{aligned} 1.0000 &\pm 0.0010 \\ 1.0000 &\pm 0.0038 \\ 1.0000 &\pm 0.0030 \\ 0.9985 &\pm 0.0011 \end{aligned}$	$\begin{array}{c} 0.9992 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 1.0025 \pm 0.0003 \\ 0.9978 \pm 0.0004 \end{array}$	0.9990 ± 0.0003 1.0001 ± 0.0003 1.0023 ± 0.0003 0.9969 ± 0.0004	0.9962 ± 0.0003 0.9972 ± 0.0004 1.0024 ± 0.0003 0.9948 ± 0.0003
	Intermediate	UH ₃ (6) Zeus (2)	1.0000 ± 0.0047 0.9997 ± 0.0008	$0.9926 \pm 0.0003 \\ 0.9948 \pm 0.0003$	0.9925 ± 0.0003 0.9945 ± 0.0004	0.9914 ± 0.0003 0.9942 ± 0.0003
	Thermal	SB-5 ORNL-10	$1.0015 \pm 0.0028 1.0015 \pm 0.0026$	$0.9943 \pm 0.0005 \\ 0.9994 \pm 0.0002$	0.9941 ± 0.0005 0.9986 ± 0.0002	$0.9963 \pm 0.0005 \\ 0.9992 \pm 0.0002$
IEU	Fast	IEU-MF-03 BIG TEN IEU-MF-04	1.0000 ± 0.0017 0.9948 ± 0.0013 1.0000 ± 0.0030	1.0026 ± 0.0003 0.9950 ± 0.0002 1.0077 ± 0.0003	1.0032 ± 0.0003 0.9953 ± 0.0002 1.0081 ± 0.0003	0.9987 ± 0.0003 1.0071 ± 0.0003 1.0038 ± 0.0003
	Intermediate	Zebra-8H	1.0300 ± 0.0025	1.0190 ± 0.0002	1.0197 ± 0.0003	1.0405 ± 0.0002
	Thermal	IEU-CT-02 (3) STACY-36	1.0017 ± 0.0044 0.9988 ± 0.0013	1.0005 ± 0.0003 0.9983 ± 0.0003	0.9997 ± 0.0003 0.9973 ± 0.0003	$1.0007 \pm 0.0003 \\ 0.9988 \pm 0.0003$
LEU	Thermal	BaW XI (2) LEU-ST-02 (2)	1.0007 ± 0.0012 0.9991 ± 0.0029	0.9997 ± 0.0003 0.9957± 0.0003	0.9977 ± 0.0003 0.9944 ± 0.0003	$0.9968 \pm 0.0003 \\ 0.9957 \pm 0.0003$
Pu	Fast	Jezebel Jezebel-240 Pu Buttons (3) Flattop-Pu THOR Pu-MF-11	$\begin{array}{c} 1.0000 \pm 0.0020 \\ 1.0000 \pm 0.0020 \\ 1.0000 \pm 0.0030 \\ 1.0000 \pm 0.0030 \\ 1.0000 \pm 0.0006 \\ 1.0000 \pm 0.0010 \end{array}$	1.0004 ± 0.0003 1.0001 ± 0.0003 0.9986 ± 0.0003 1.0006 ± 0.0003 1.0081 ± 0.0003 0.9986 ± 0.0003	$\begin{array}{c} 1.0004 \pm 0.0003 \\ 1.0001 \pm 0.0003 \\ 0.9986 \pm 0.0003 \\ 1.0008 \pm 0.0003 \\ 1.0081 \pm 0.0003 \\ 0.9986 \pm 0.0003 \end{array}$	$\begin{array}{c} 0.9975 \pm 0.0003 \\ 0.9979 \pm 0.0003 \\ 0.9962 \pm 0.0003 \\ 1.0013 \pm 0.0003 \\ 1.0062 \pm 0.0003 \\ 0.9970 \pm 0.0003 \end{array}$
	Intermediate	HISS/HPG	1.0000 ± 0.0110	1.0111 ± 0.0005	1.0111 ± 0.0005	1.0104 ± 0.0003
	Thermal	PNL-33 PNL-2	1.0024 ± 0.0021 1.0000 ± 0.0065	1.0057 ± 0.0003 1.0039 ± 0.0010	$1.0053 \pm 0.0007 \\ 1.0039 \pm 0.0010$	1.0029 ± 0.0003 1.0033 ± 0.0005

resonance parameters for 238 U produces a significantly better value for $k_{\rm eff}$ for B&W XI (2), a lattice of LEU fuel pins in water, and ORNL-11, an unreflected sphere of uranyl nitrate solution enriched in 233 U.

At the same time, the preliminary ENDF/B-VII data produce worse results for thermal lattices of ²³³U and HEU pins in water (SB-2½ and SB-5, respectively), for the bare IEU sphere (IEU-MF-03) and the IEU sphere reflected by graphite (IEU-MF-04), for a plutonium sphere reflected by thorium (THOR), and for a MOX lattice in water (PNL-33). Furthermore, k_{eff} for

the uranium cases with intermediate spectra remains substantially underpredicted, while k_{eff} for the plutonium case with an intermediate spectrum (HISS/HPG) continues to be significantly over-predicted.

In conclusion, preliminary ENDF/B-VII data for the uranium isotopes and ²³⁹Pu produce improvements for most of the cases with fast spectra, BIG TEN, and the lattice of LEU fuel pins in water. However, improvements still are needed in some areas, particularly those cases with intermediate spectra.

REFERENCES

- International Handbook of Evaluated Criticality Safety Benchmark Experiments, OECD Nuclear Energy Agency report NEA/NSC/DOC(95)03, September 2003 Edition.
- X-5 Monte Carlo Team, "MCNP A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory," LA-UR-03-1987, Los Alamos National Lab. (April 2003).